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(5194) Karl Christe (ERC) *et al.*, "Studies on the Generation of the Pentazole Anion and Singlet-Delta Molecular Oxygen"

(Statement A)

AFOSR Molecular Dynamics Conference
(Boston, MA, 20 May 2002) (Deadline: ASAP – 19 May 2002)

Studies on the Generation of the Pentazole Anion and Singlet-Delta Molecular Oxygen

Karl O. Christe, William W. Wilson, Ashwani Vij, Vandana Vij, Angelo Alfano, Robert Corley, Jerry A. Boatz, Stefan Schneider, Thorsten Schroer, Ross Wagner, Michael Gerken, Ralf Haiges, and James Pavlovich

ERC and Propulsion Sciences and Advanced Concepts Division, Air Force Research Laboratory Edwards Air Force Base, CA 93524, Loker Research Institute, University of Southern California, Los Angeles, CA 90089, and Department of Chemistry, University of California, Santa Barbara, CA 93106

karl.christe@edwards.af.mil

Under combined DARPA, AFOSR and NSF sponsorship, we have discovered in 1999 the novel polynitrogen cation, N_5^+. We have successfully prepared and chararacterized the $N_5^+AsF_6^-$, $N_5^+SbF_6^-$, $N_5^+Sb_2F_{11}^-$, $N_5^+(BCF_3)_4^-$, $N_5^+SnF_5^-$, and $(N_5^+)_2SnF_6^{2-}$ salts. However attempts to prepare $N_5^+N_3^-$ were unsuccessful due to the low first ionization potential of N_3^-. Theoretical calculations predict that the pentazole anion, N_5^-, should possess a significantly higher first ionization potential and a good barrier towards decomposition, and numerous research groups are actively pursuing the synthesis of this interesting anion. In this presentation, we report the first experimental detection of the pentazole anion.

Singlet delta oxygen plays an important role in the COIL laser that is a cornerstone of the missile defense system. The presently used singlet-delta oxygen generation system suffers from liquid phase quenching and the instability of basic hydrogen peroxide. These drawbacks can be overcome by a novel gas-solid system. It is based on commercially available stable starting materials and avoids liquid phase quenching. This system, which was developed under DARPA sponsorship, will be briefly described.